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In Situ X-ray Diffraction Study of Phase Diagram of Germanium at Pressures up to 11 GPa and Temperatures up to 950 K

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Beamline(s): X17B1

Introduction: While phase transitions in Ge at high pressures have been intensively studied at room temperature, the high-temperature region of its phase diagram has been investigated incompletely and mainly by resistance measurements [1,2]. In this work we studied Ge phase transitions and melting by in situ X-ray diffraction method, which allows much more precise pressure measurements and detailed investigation of high-pressure phases structure.

Methods and Materials: Three X-ray diffraction experiments were performed using a DIA-type cubic anvil apparatus and T-Cup high-pressure system. An energy-dispersive x-ray method was employed using white radiation at beamline X17B of NSLS. In all experiments, NaCl was used as an internal pressure standard, and temperature was measured by a W/Re25%-W/Re3% thermocouple. In the course of the experiments, diverse P-T paths were used in order to study Ge_I – Ge_{II} transition at various temperatures and melting of Ge at different pressures.

Results: In situ X-ray measurements enabled us to define more exactly a phase diagram for germanium in the pressure range 0 – 11 GPa. The Ge_I – Ge_{II} – Ge_L triple point is close to 843 K and 8.7 GPa (Fig. 1). At room temperature the onset of the Ge_I – Ge_{II} transition in hydrostatic conditions was found at 11.1 GPa and at 473 K – at 9.7 GPa. The volume effects of the Ge_I – Ge_{II} transition were calculated at these points. The Ge_{II} phase has large anisotropy of thermal expansion: the average values of α_t^a and α_t^c in the temperature interval 298 – 873 K are $(12 \pm 1)\times10^{-6}$ K^{-1} and $(22 \pm 2)\times10^{-6}$ K^{-1}, respectively. The Ge_{II} – (Ge_{III} + Ge_{IV}) transition occurs only as a result of decompression at temperatures below 473 K. Phases Ge_{III} and Ge_{IV} are metastable forms of germanium and transform into Ge_I at temperatures 473 – 623 K even in the proximity of Ge_I – Ge_{II} equilibrium boundary.

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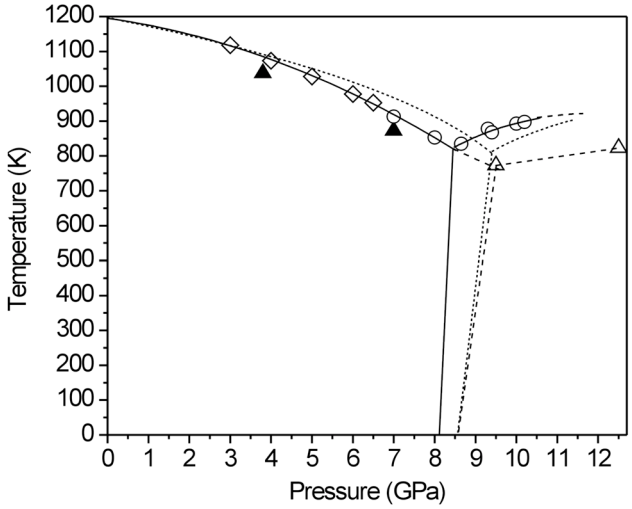

Figure 1. P-T phase diagram of germanium: circles, solid line – present work, dotted line - Brazhkin et. al. [2], dashed line – Cannon [3], diamonds – Vaidya et. al. [4], closed triangles – Bundy [1], opened triangles – Bundy (Cannon [3]).